

91) Expressions for Fermi energy μ .

(i) At $T = 0$

N particles in volume V

Number particles
with $\epsilon \rightarrow \epsilon + d\epsilon$ = Number states
 $\epsilon \rightarrow \epsilon + d\epsilon$ \times Prob of
state occupation

$$n(\epsilon) d\epsilon = g(\epsilon) d\epsilon \times f(\epsilon)$$

$$N = \int_0^{\infty} n(\epsilon) d\epsilon = \int_0^{\infty} g(\epsilon) d\epsilon \times f(\epsilon)$$

Recall $g(\epsilon) d\epsilon = 4\pi V \left(\frac{2m}{h^2} \right)^{3/2} \epsilon^{1/2} d\epsilon$

$$N = \int_0^{\infty} 4\pi V \left(\frac{2m}{h^2} \right)^{3/2} \epsilon^{1/2} d\epsilon \cdot f(\epsilon)$$

but $f(\epsilon) = 1 \quad \epsilon < \mu$

$$f(\epsilon) = 0 \quad \epsilon > \mu$$

Thus

$$N = 4\pi V \left(\frac{2m}{h^2} \right)^{3/2} \int_0^{\mu} \epsilon^{1/2} d\epsilon$$

(92)

gives
$$N = 4\pi V \left(\frac{2m}{h^2} \right)^{3/2} \cdot \frac{2}{3} \mu^{3/2}$$

$$\mu = \left(\frac{h^2}{2m} \right) \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

Strictly this μ should be denoted
 $\mu(0) \leftarrow$ evaluated at $T=0$.

Alternative method for $\mu(0)$.

Recall k space spanned by quantum states with $k_x = \frac{2\pi}{L} \cdot n_x$, $k_y = \frac{2\pi}{L} n_y \dots$

and particle kinetic energy ϵ given by

$$\epsilon = \frac{h^2 k^2}{2m}$$

Corresponding to Fermi energy μ is k_F

where
$$\mu = \frac{h^2 k_F^2}{2m}$$

(93)

where $k < k_F$ states filled

$k > k_F$ states empty

Then

N = number of filled states

$$N = 2 \times \frac{4\pi k_F^3}{3} \times \frac{1}{(2\pi/L)^3}$$

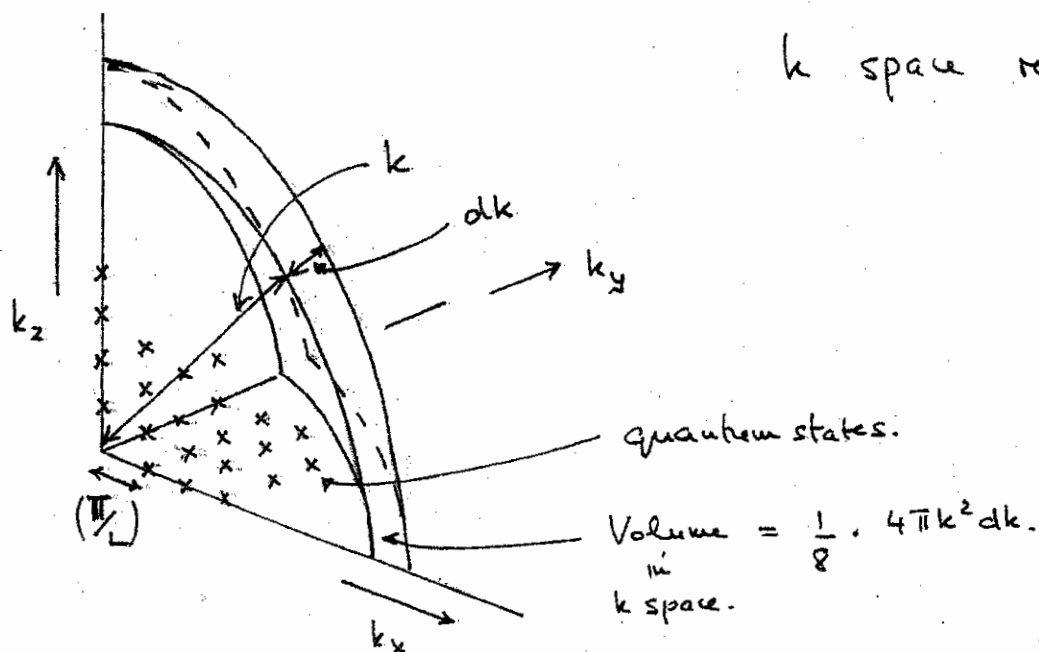
\uparrow and \downarrow \downarrow volume of k space \downarrow volume of k space per state.

$$N = \frac{8\pi k_F^3}{3} \cdot \frac{V}{(2\pi)^3}$$

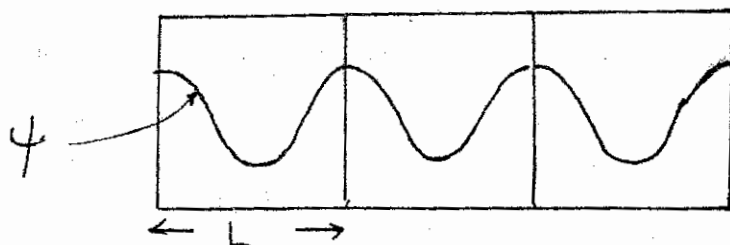
$$k_F^3 = \frac{3\pi^2 N}{V}$$

$$\mu(0) = \frac{\hbar^2 k_F^2}{2m} = \left(\frac{\hbar^2}{2m} \right) \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

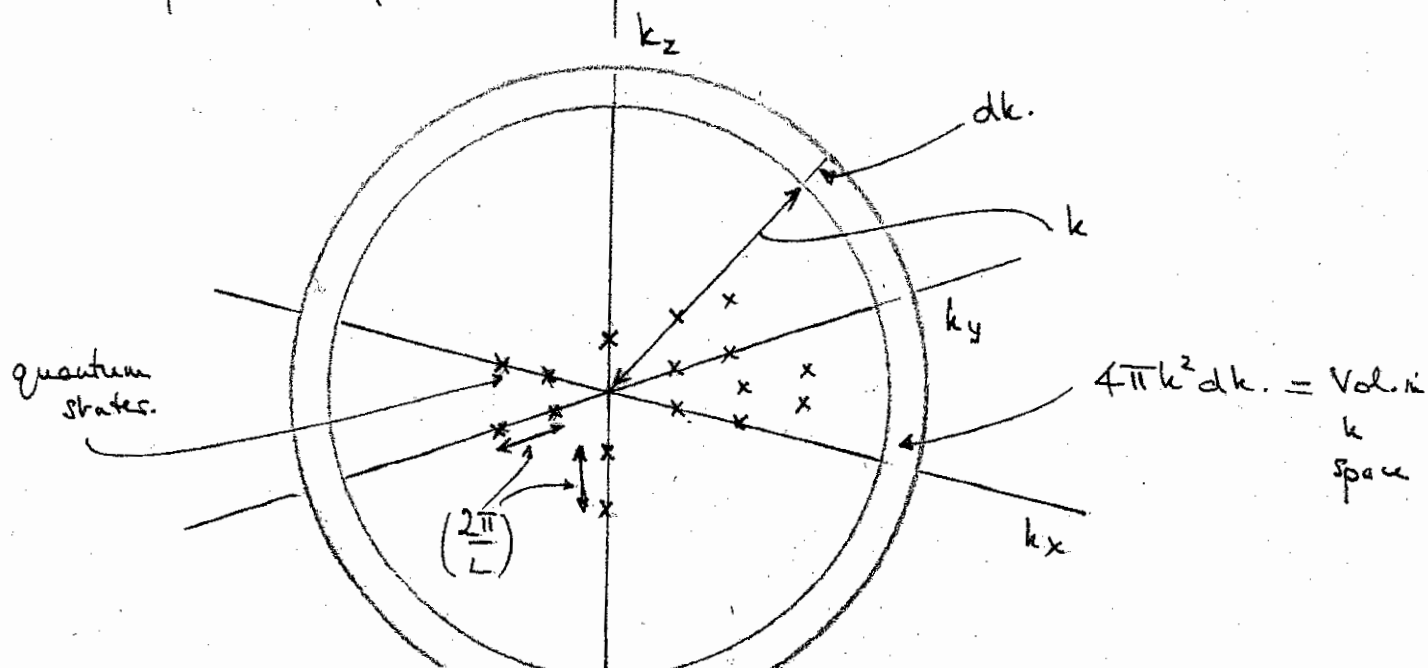
Standing wave boundary conditions.



Periodic Boundary conditions.



k space representation



(94)

Classical and quantum limits.

Combining
$$A = \frac{N}{V} \left(\frac{h^2}{2\pi m k T} \right)^{3/2}$$

and
$$\mu(0) = \left(\frac{h^2}{2m} \right) \left(\frac{3\pi^2 N}{V} \right)^{2/3} = k T_F$$

get
$$A = \frac{8}{3\sqrt{\pi}} \left(\frac{T_F}{T} \right)^{3/2}$$

Classical condition

$$A \ll 1 \quad \text{equivalent to} \quad T \gg T_F$$

Quantum condition

$$A \gg 1 \quad \text{equivalent to} \quad T \ll T_F$$

Where are actual systems on this scale?

1. Conduction electrons in copper.

For Cu
$$\frac{N}{V} = 8.5 \times 10^{28} \text{ m}^{-3}$$

Variation of Fermi energy μ with temperature T .

Q. Does μ vary with T ?

A. Yes - but in quantum (degenerate) limit - the variation is small.

Analysis.

Recall
$$N = \int_0^{\infty} g(\epsilon) \cdot f(\epsilon) d\epsilon$$

Procedure - do this integration (i) at $T=0$
(ii) at $T>0$

and equate.

Write $g(\epsilon) = C\epsilon^{1/2}$ where $C = 4\pi V \left(\frac{2m}{h^2} \right)^{3/2}$

(i) At $T=0$

$$N = \int_0^{\mu(0)} C\epsilon^{1/2} f(\epsilon) d\epsilon = \int_0^{\mu(0)} C\epsilon^{1/2} d\epsilon = \frac{2}{3} C [\mu(0)]^{3/2}$$

(ii) At $T>0$

$$N = \int_0^{\infty} C\epsilon^{1/2} f(\epsilon) d\epsilon$$

To do this integral use method of Guenault Appendix 3.

Write integral in form
$$N = \int_0^{\infty} \left(\frac{dF}{d\epsilon} \right) f(\epsilon) d\epsilon$$
$$= [F(\epsilon)f(\epsilon)]_0^{\infty} - \int_0^{\infty} F(\epsilon) \left(\frac{df}{d\epsilon} \right) d\epsilon$$

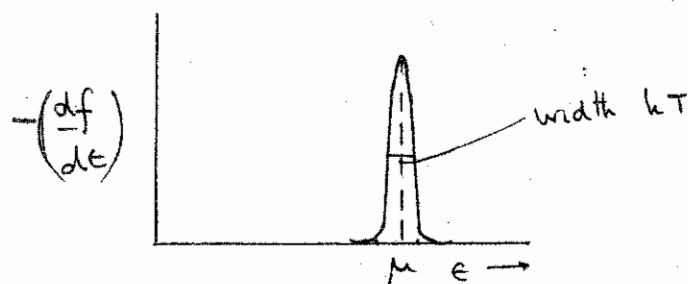
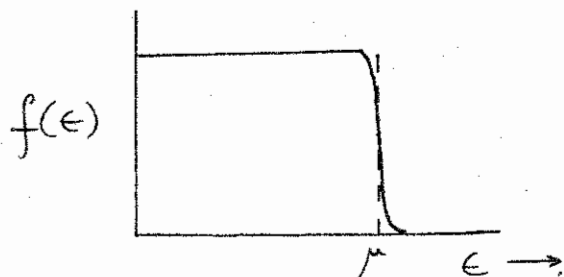
In our case $\left(\frac{dF}{d\epsilon}\right) = C\epsilon^{1/2}$

$$F(\epsilon) = \frac{2}{3} C \epsilon^{3/2}$$

Then $N = \left[\frac{2}{3} C \epsilon^{3/2} f(\epsilon) \right]_0^\infty - \int_0^\infty \frac{2}{3} C \epsilon^{3/2} \left(\frac{df}{d\epsilon}\right) d\epsilon$

↓

$$N = 0 - \int_0^\infty \frac{2}{3} C \epsilon^{3/2} \left(\frac{df}{d\epsilon}\right) d\epsilon$$



See from graphs that integrating with $-(\frac{df}{d\epsilon})$ picks out $\frac{2}{3} C \epsilon^{3/2}$

at $\epsilon = \mu$. - due to

finite width kT - there is

correction term.

Gives

Quantum Appendix 3

$$N = \frac{2}{3} C \mu^{3/2} + \frac{\pi^2}{6} (kT)^2 \left(\frac{d^2 F}{d\epsilon^2}\right)_{\epsilon=\mu}$$

Thus $N = \frac{2}{3} C \mu^{3/2} + \frac{\pi^2}{6} \cdot (kT)^2 \cdot \frac{1}{2} \frac{C}{\mu^{1/2}}$

Equate $T=0$ and $T \neq 0$ integrals for N

$$\frac{2}{3} C \mu(0)^{3/2} = \frac{2}{3} C \mu^{3/2} + \frac{\pi^2}{12} (kT)^2 \frac{C}{\mu^{1/2}}$$

$$\mu(0)^{3/2} = \mu^{3/2} \left[1 + \frac{3}{2} \cdot \frac{\pi^2}{12} \cdot \left(\frac{kT}{\mu}\right)^2 \right]$$

$$\mu = \mu(0) \left[1 + \frac{3}{2} \cdot \frac{\pi^2}{12} \cdot \left(\frac{kT}{\mu}\right)^2 \right]^{-2/3}$$

Small since $kT \ll \mu$

$$\mu = \mu(0) \left[1 - \frac{\pi^2}{12} \left(\frac{kT}{\mu}\right)^2 + \dots \right]$$

Small variation of μ with T

(96)

Variation of Fermi energy μ with
temperature T see sheets.

Thermodynamic quantities.

Energy U

$$U = \sum_i n_i \epsilon_i$$

In gas $U = \int_0^{\infty} \epsilon g(\epsilon) f(\epsilon) d\epsilon$

At $T=0$

$$U(0) = \int_0^{\mu(0)} \epsilon \cdot C \epsilon^{1/2} d\epsilon = \int_0^{\mu} C \epsilon^{3/2} d\epsilon$$

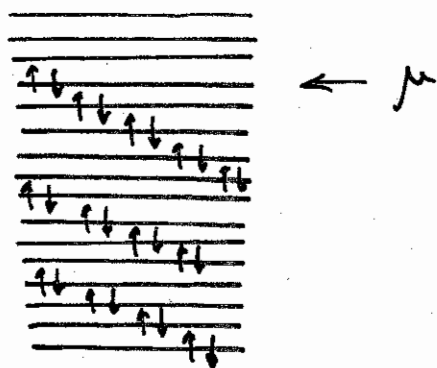
$$U(0) = \frac{2}{5} C \mu^{5/2}$$

But above $N = \frac{2}{3} C \mu^{3/2}$

$$\text{Thus } U(0) = \frac{3}{5} N \mu.$$

97

$U(0) = \frac{3}{5} N \mu$ is very large zero point energy — because of Pauli principle not allowing more than \uparrow and \downarrow fermions in same state.



— fermions cannot all go to lowest states.

For $T > 0$ but $T \ll T_F$

$$U = \int_0^{\infty} \epsilon \cdot C \epsilon^{1/2} f(\epsilon) d\epsilon$$

Similar integration to that for Fermi energy gives

$$U = U(0) + U(\text{thermal})$$

$$U = \frac{3}{5} N \mu + \frac{\pi^2}{6} (kT)^2 g(\mu)$$

↓
Zero point energy

↓
thermal energy

$g(\mu)$ = density of states at Fermi energy.

48

Density of states at fermi energy - see diagram on sheet.

Understand form of $U(\text{thermal})$ from

- (i) Only states that can be excited at temp T lie within energy kT of μ
- (ii) Number of particles involved $= g(\mu) \cdot kT$
Excitation energy / particle $= kT$

Thermal excitation energy $U(\text{th}) \approx (kT)^2 g(\mu)$

Graph of U vs T - see sheet.

For $T \gg T_F$

Classical limit.

$$U \rightarrow \frac{3}{2} NkT.$$

59 Heat capacity C_V

$$C_V = \left(\frac{\partial U}{\partial T} \right)_V = \frac{\partial}{\partial T} \left[\frac{3}{5} N \mu + \frac{\pi^2}{6} (kT)^2 g(\mu) \right]$$

$$C_V = \frac{\pi^2}{3} k^2 T g(\mu)$$

Graph of C_V vs T — see sheet

Points

1. As $T \rightarrow 0$ $C_V \rightarrow 0$

2. In exptl range for conduction electrons

C_V is (i) small

(ii) \propto Temperature T .

3. For $T \gg T_F$ — classical limit

$$C_V = \frac{\partial U}{\partial T} \rightarrow \frac{\partial}{\partial T} \left(\frac{3}{2} N k T \right) = \frac{3}{2} N k.$$

4. For $g(\epsilon) = C \epsilon^{1/2}$ — see diagram

$$g(\mu) = \frac{3N}{2}$$

(100)

Then in quantum region can write

$$C_V = \frac{\pi^2}{3} k^2 T g(\mu) = \frac{\pi^2}{3} k^2 T \frac{3N}{2\mu}$$

$$C_V = \frac{\pi^2}{3} \left(\frac{3}{2} Nk \right) \cdot \left(\frac{kT}{\mu} \right)$$

↓
classical \times fermifunction (small).

Pressure P .

First Law $dU = TdS - pdV$

For constant S $P = - \left(\frac{\partial U}{\partial V} \right)_S$

Quantum limit

$$U = \sum_i n_i \epsilon_i$$

$$P = - \left(\frac{\partial U}{\partial V} \right)_S = - \sum_i n_i \left(\frac{\partial \epsilon_i}{\partial V} \right)$$

n_i const at const S

(101)

Recall $\epsilon = \frac{\hbar^2 k^2}{2m}$

$$k = \frac{2\pi n}{L}$$

$$k^2 \propto L^{-2} \quad \text{or} \quad V^{-2/3}$$

$$\text{Thus } \epsilon \propto V^{-2/3} = KV^{-2/3}$$

$$\text{Hence } \left(\frac{\partial \epsilon}{\partial V} \right) = -\frac{2}{3} KV^{-5/3} \equiv -\frac{2}{3} \frac{\epsilon}{V}$$

$$\text{Then } p = - \sum \left(-\frac{2}{3} \right) \frac{n_i \epsilon_i}{V}$$

$$p = \frac{2}{3} \frac{U}{V}$$

Points

1. This large pressure at quantum limit due to large $U(0)$ - keeps neutron stars stable against gravitational force

(102)

2. At classical limit $T \gg T_F$

$$p \rightarrow \frac{NkT}{V} \quad - \text{ see sheet.}$$

Entropy S .

Tedious to calculate

Know that as $T \rightarrow 0$

$$S \rightarrow 0$$

with particles condensing into lowest set of 'tower block' states.

Conduction electrons.

All exptl data occur in range $T \ll T_F$

Thus predicted properties in quantum

limit of graphs of $\left. \begin{array}{l} U \\ C_v \\ p \end{array} \right\} \text{ versus } T.$

103

Magnetisation of conduction electrons.

— see sheet.

Magnetisation M of conduction electrons.

M is magnetic moment / m^3 developed by conduction electrons when magnetic field B is applied to the piece of metal.

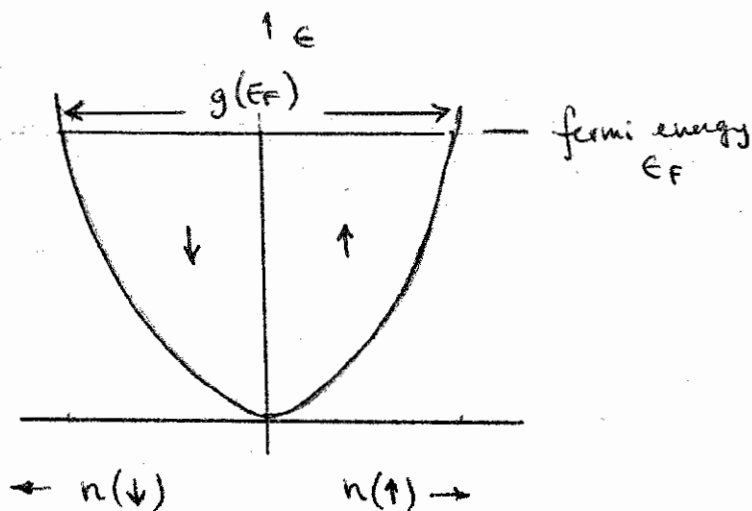
In field B each spin $\frac{1}{2}$ electron has to orient spin either parallel to B or opposite to B

$$\text{magnetic energy} = -\mu B$$

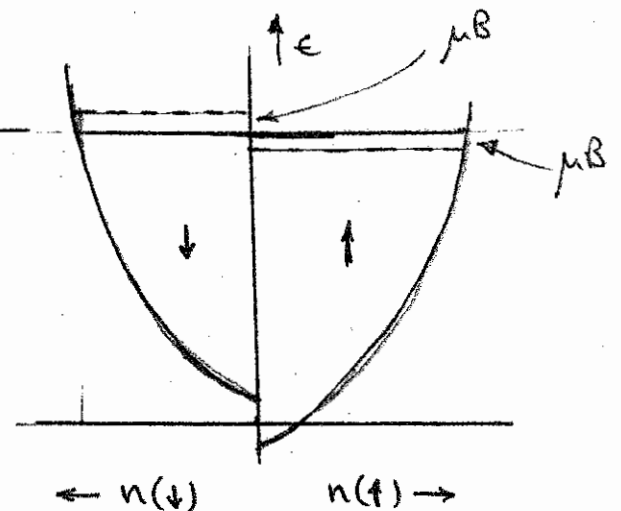
$$\text{magnetic energy} = +\mu B$$

where μ = magnetic moment of electron (1 Bohr magneton)

Electron states. — use ϵ_F as fermi energy.



Zero field.



Field $B \uparrow$

$$\text{Magnetic moment } M = [n(\uparrow) - n(\downarrow)] \mu.$$

When field B applied $\frac{1}{2} g(\epsilon_F) \cdot \mu B$ electrons

Then $M = \frac{1}{2} g(\epsilon_F) \mu_B \cdot 2\mu^*$

For $g(\epsilon_F) = \frac{3N}{2\epsilon_F}$

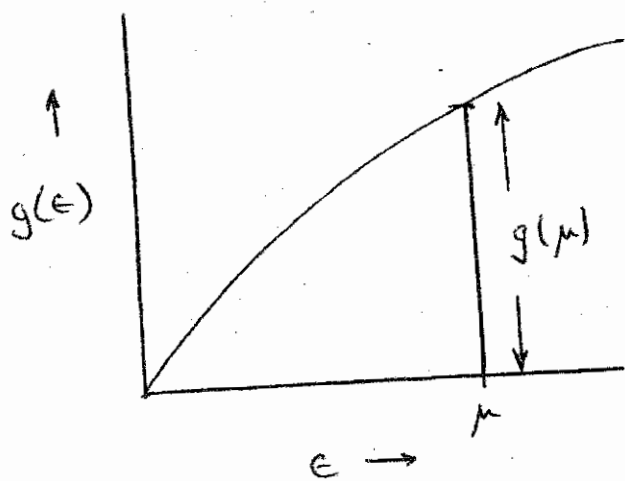
$$M = \frac{3N}{2\epsilon_F} \mu^2 B.$$

Predicts

1. Magnetic susceptibility $\chi = \frac{\mu_0 M}{B}$ is independent of temperature.
2. $\chi \propto$ density of states at fermi energy.

These confirmed by expt.

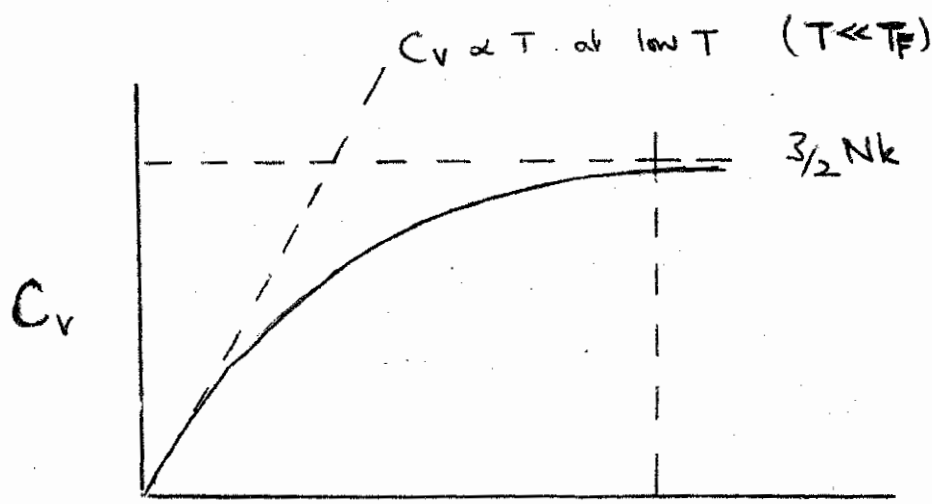
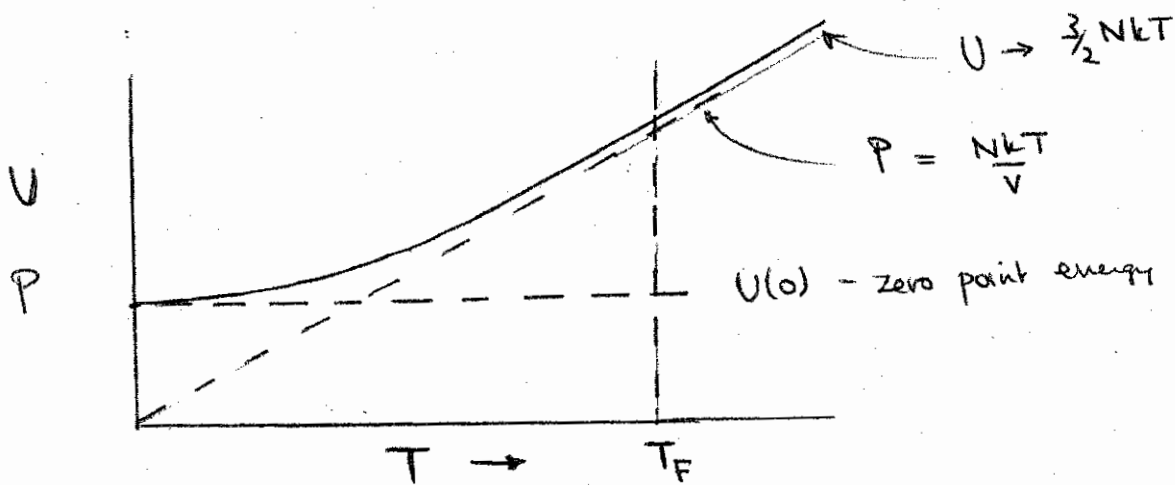
Density of states at the Fermi energy $g(\mu)$



For $g(\epsilon) = C\epsilon^{1/2}$
 $N = \frac{2}{3} C \mu^{3/2} \quad (T=0)$

Then $g(\mu) = C\mu^{1/2} = \frac{3N}{2\mu}$

Energy U versus T
 Pressure P versus T



Statistical Mechanics Theory

N identical particles
Volume V
Thermal equilibrium at temperature T
Weak interactions

Particles distinguishable by position in solid

Gas particles in macroscopic box.
Particles indistinguishable

occupation number

$f \gg 1$

occupation number

$f \ll 1$

$$n_j = \frac{N}{Z} \exp(-\epsilon_j/kT)$$

$$Z = \sum_j \exp(-\epsilon_j/kT)$$

Quantum region
Behaviour depends whether $\psi(1,2)$ symmetric or antisymmetric under particle exchange

Classical region
Maxwell Boltzmann statistics

$$f(\epsilon) = \frac{N}{Z} \exp(-\epsilon/kT)$$

$$Z = V \left(\frac{2\pi mkT}{h^2} \right)^{3/2}$$

$\psi(1,2)$ antisymmetric

$\psi(1,2)$ symmetric

Fermi Dirac statistics

$$f(\epsilon) = \frac{1}{\exp(\epsilon - \mu/kT) + 1}$$

μ = Fermi energy

Bose-Einstein statistics

$$f(\epsilon) = \frac{1}{\exp(\epsilon/kT) - 1}$$

basic theory

basic theory

basic theory

basic theory

Excitations in localised atoms

Conduction electrons
Liquid He^3
 He^3/He^4 liquid mixtures

Radiation in enclosure
Phonons in solids
Superconductors
Liquid He^4

normal gases

Boson gases.

At low temperature

- fermions show "tower block" occupancy of energy states because of Pauli principle.
- bosons not subject to Pauli principle can show heavy population - "condensation into" the ground state.

Can cause dramatic macroscopic effects.

Bose Einstein distribution

$$f(\epsilon) = \frac{1}{B \exp(\epsilon/kT) - 1}$$

Parameter B determined from

$$\sum_i n_i = N$$

(105)

Range of values of B .

$f(\epsilon)$ cannot be negative

As $\epsilon \rightarrow 0$ giving $\exp(\epsilon/kT) \rightarrow 1$

Sets range $1 < B$

(i) For conditions where $B \gg 1$ have

Classical region

B -Einstein distribⁿ \longrightarrow Maxwell Boltzmann

$$\frac{1}{B \exp(\epsilon/kT) - 1} \longrightarrow A \exp(-\epsilon/kT)$$

(ii) For $B \rightarrow 1$

Achieved at low temperature

Quantum region

In theory above - have determined B from

$$N = \sum_i n_i = \int_0^{\infty} g(h) f(h) dh \quad \text{or} \quad \int_0^{\infty} g(\epsilon) f(\epsilon) d\epsilon$$

(106)

Boson case

$$N = \int_0^{\infty} g(k) dk f(k)$$

$$= \int_0^{\infty} \frac{4\pi V k^2 dk}{(2\pi)^3} \cdot \frac{1}{\left[\exp\left(\frac{\hbar^2 k^2}{2mkT}\right) - 1 \right]}$$

where $\epsilon = \frac{\hbar^2 k^2}{2m}$

Putting $y^2 = \frac{\hbar^2 k^2}{2mkT}$

$$y dy = \frac{\hbar^2}{2mkT} \cdot k dk$$

$$y^2 dy = \left(\frac{\hbar^2}{2mkT} \right)^{3/2} k^2 dk$$

$$N = \frac{4\pi V}{(2\pi)^3} \left(\frac{2mkT}{\hbar^2} \right)^{3/2} \int_0^{\infty} \frac{y^2 dy}{\left[\exp(y^2) - 1 \right]}$$

$$N = \frac{4}{\sqrt{\pi}} \cdot V \left(\frac{2\pi mkT}{h^2} \right)^{3/2} \int_0^{\infty} \frac{y^2 dy}{\left[\exp(y^2) - 1 \right]}$$



$Z \equiv \text{partition f}^n.$

Thus.

$$N = Z F(B)$$

where
$$F(B) = \frac{4}{\sqrt{\pi}} \int_0^{\infty} \frac{y^2 dy}{B \exp(y^2) - 1}$$

Graph of $F(B)$ vs B — see sheet.

Previously have defined degeneracy parameter

A where

$$A = \frac{N}{Z} = \left(\frac{N}{V} \right) \left(\frac{h^2}{2\pi m k T} \right)^{3/2}$$

Find

$A \ll 1$ classical region

$A \approx 1$ changeover

$A > 1$ quantum region

Since both $= N/Z$

$$A = F(B)$$

Problems for theory.

Values of T , $(\frac{N}{V})$ determine A

A increases when T decreases
 $(\frac{N}{V})$ increases.

But $F(B)$ cannot exceed 2.612

Since B must > 1

In terms of relation

$$N = \underbrace{Z \cdot F(B)}$$

can only represent $2.612 Z$
 particles — may be
 less than N .

What has gone wrong?

Relation $N = \int_0^{\infty} g(k) f(k) dk$

assumes a smooth variation in population
 of states

109

At very low temperature - very large numbers of bosons go into ground state
Variation in population between ground state and excited states is not smooth.

Illustration — see sheet.

This excess population of ground state called Bose-Einstein Condensation. — occurs for temperatures T below a critical temp T_B .

Critical condition

$$B = 1 \quad F(B) = 2.612$$

Then

$$2.612 = \left(\frac{N}{V} \right) \left(\frac{h^2}{2\pi m k T_B} \right)^{3/2}$$

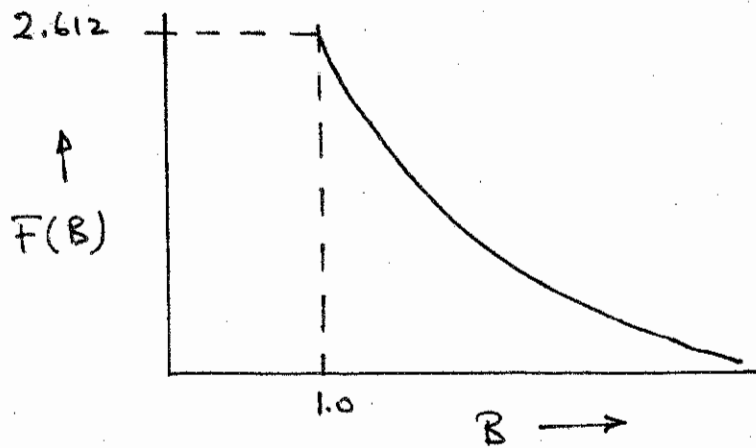
gives critical temp T_B as

$$T_B = \left(\frac{h^2}{2\pi m k} \right) \left(\frac{N}{2.612 V} \right)^{2/3}$$

Bose - Einstein gas.

Graph of $F(B)$ vs B

where
$$F(B) = \frac{4}{\sqrt{\pi}} \int_0^\infty \frac{y^2 dy}{B \exp(y^2) - 1}$$

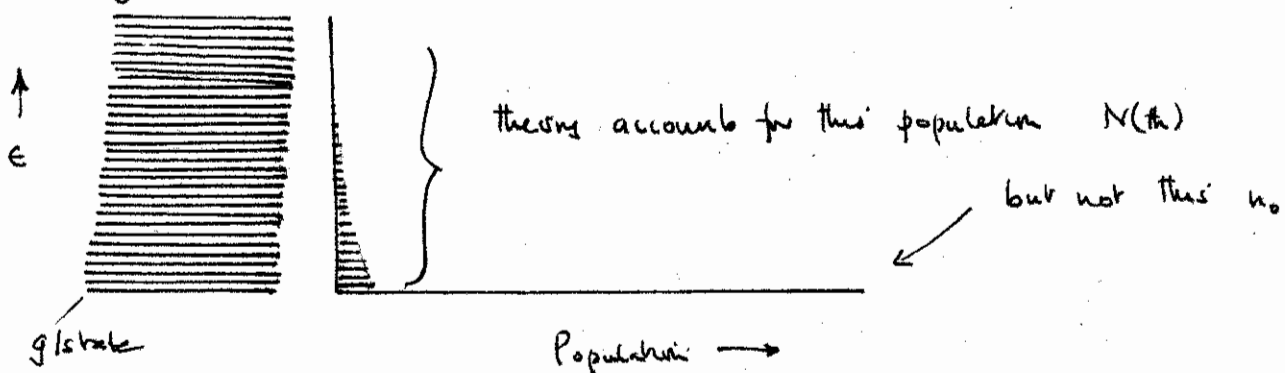


Points

- (i) For $B \gg 1$ $F(B) \rightarrow \frac{1}{B}$
- (ii) $F(B)$ only defined in range $1 < B$
- (iii) For $B = 1$ $F(B) = 2.612$.

Population of states by bosons at low temperature

Quantum states



(110)

Population in ground state

Total number of particles = Number in ground state + Number in excited states

$$N = n_0 + N(\text{th})$$

Degeneracy of g/state = g_0

$$n_0 = g_0 \cdot \frac{1}{(B-1)}$$

$N(\text{th})$ — given by distribution.

For temperatures $T > T_B$

No B-E condensation

$$B > 1$$

n_0 — not large

$$N(\text{th}) = V \left(\frac{2\pi m k T}{h^2} \right)^{3/2} F(B)$$

For temperatures $T < T_B$

$$N(\text{th}) = Z \times 2.612 = 2.612 V \left(\frac{2\pi m k T}{h^2} \right)^{3/2}$$